

3. AIR ALGORITHMS

In this chapter, the algorithms for the horizontal transport of chemical species between air compartments and those for diffusion/volatilization between air compartments and surface water are presented. A description of deposition from air compartments to surface water can be found in Chapter 4, and a description of the transport processes between air compartments and soil can be found in Chapter 5. The text box on the next page provides a summary of the T-factor algorithms developed in this chapter and definitions of the parameters used in those algorithms.

3.1 AIR-TO-AIR ALGORITHMS

For a given wind speed and direction, there are two types of transfer processes that account for the majority of chemical mass that moves from one air compartment to another:

- Advective transfer (bulk) due to the component of the wind vector normal to the boundary between the compartments; and
- Dispersive transfer (bulk) calculated from the component of the wind vector parallel to the boundary between the compartments.

The total transfer factor from one air compartment to an adjacent air compartment is the sum of these two transfers.

The current TRIM.FaTE library incorporates only the advective transfer due to the wind vector normal to the boundary between compartments. This is because of the complexity and technical challenges related to the representation of dispersive transfers in a compartment-based modeling system such as TRIM.FaTE. Note that diffusion between air compartments is considered negligible and thus is not included in TRIM.FaTE.

Let *Air_Rcv* and *Air_Send* denote the adjacent receiving and sending air compartments. If the boundary between the two air compartments is composed of *n* distinct line segments, then the transfer factor from the sending to the receiving air compartment is calculated as:

$$T_{Air_Send \rightarrow Air_Rcv}^{adv} = \frac{1}{V_{Send}} \times \sum_{i=1}^n A_i \times (u_i^{(D)} + u_i^{(L)}) \quad (\text{Eq. 3-1})$$

where:

- V_{Send} = volume of the sending air compartment (m³);
- A_i = interfacial area across *i*th boundary (m²);
- $u_i^{(D)}$ = direct (D) advective wind velocity across the *i*th boundary (m/day); and
- $u_i^{(L)}$ = lateral (L)/dispersive wind velocity across the *i*th boundary (m/day).

The direct wind flow across an air compartment boundary (notation $u_i^{(D)}$ is used above) is calculated by finding the projection of the wind vector onto the normal vector to the boundary between the air compartments.

Summary of Transfer Factors for Air in TRIM.FaTE

AIR ADVECTION

Air compartment to air compartment: (TF 3-1)

$$T_{Air_Send \rightarrow Air_Rcv}^{adv} = \frac{1}{V_{Air_Send}} \times \sum_{i=1}^n A_i \times (u_i^{(D)})$$

AIR DIFFUSION/VOLATILIZATION

Diffusion from air compartment to surface water compartment: (TF 3-2)

$$T_{Air \rightarrow SW}^{dif} = \frac{A_{SWA}}{V_{Air}} \times \frac{k_v}{H/(R \times T)} \times f_{MV}$$

Volatilization from surface water compartment to air compartment: (TF 3-3)

$$T_{SW \rightarrow Air}^{vol} = \frac{A_{SWA}}{V_{SW}} \times k_v \times f_{ML}$$

LIST OF SYMBOLS USED IN AIR TRANSFER FACTOR ALGORITHMS

V_{Air_Send}	=	volume of the sending air compartment (m ³).
A_i	=	interfacial area across <i>i</i> th boundary (m ²).
$u_i^{(D)}$	=	direct advective wind velocity across the <i>i</i> th boundary (m/day).
A_{SWA}	=	interfacial area between the surface water and air compartments (m ²).
V_{Air}	=	volume of air compartment (m ³).
k_v	=	volatilization transfer rate (m/day).
H	=	Henry's law coefficient for the air-water partitioning of the chemical (atm-m ³ /mole).
R	=	universal gas constant (8.206x10 ⁻⁵ atm-m ³ /mole °K).
T	=	water temperature (°K).
f_{MV}	=	fraction of chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the compartment that is air (<i>i.e.</i> , excluding particles) (unitless).
V_{SW}	=	volume of the surface water compartment (m ³).
f_{ML}	=	fraction of chemical mass in the surface water compartment that is dissolved in water divided by volume fraction of the surface water compartment that is water (<i>i.e.</i> , excluding suspended sediments and algae) (unitless).

Let $P_1 = (x_1, y_1)$ and $P_2 = (x_2, y_2)$ be the points defining the line that is the projection of the boundary onto the *xy*-plane (*i.e.*, the view from above the vertical plane defining the boundary). It is assumed that the points P_1 and P_2 are ordered so that the receiving compartment is on the right side of the directed line segment starting at P_1 and ending at P_2 . The unit vector \bar{v} perpendicular to this line segment that is in the direction of the receiving compartment is given by:

$$\vec{v} = \frac{1}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times \langle y_2 - y_1, -(x_2 - x_1) \rangle = \langle \sin \varphi, \cos \varphi \rangle \quad (\text{Eq. 3-2})$$

where:

φ = the angle measured clockwise from due north.

If the wind is blowing with speed u toward the direction ϑ (measured clockwise from due north), then the wind vector, denoted by \vec{w} , can be written:

$$\begin{aligned} \vec{w} &= \langle u \times \cos(\pi/2 - \vartheta), u \times \sin(\pi/2 - \vartheta) \rangle \\ &= u \langle \sin \vartheta, \cos \vartheta \rangle \end{aligned} \quad (\text{Eq. 3-3})$$

The projection of the wind vector \vec{w} onto \vec{v} is just the dot product ($\vec{w} \cdot \vec{v}$) of the two vectors, which is given by:

$$\begin{aligned} \vec{w} \cdot \vec{v} &= \frac{u}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times [(y_2 - y_1) \sin \vartheta - (x_2 - x_1) \cos \vartheta] \\ &= u [\sin \vartheta \sin \varphi + \cos \vartheta \cos \varphi] \\ &= u \cos(\vartheta - \varphi) \end{aligned} \quad (\text{Eq. 3-4})$$

Since \vec{v} is a unit vector, the dot product in this case is the component of the vector \vec{w} in the direction of \vec{v} . The wind flow rate from the sending compartment to the receiving compartment is defined to be the dot product if it is positive; otherwise, it is zero. In other words:

$$\text{Wind speed perpendicular to compartment boundary} = u_{\perp} = \max\{0, u \cos(\vartheta - \varphi)\} \quad (\text{Eq. 3-5})$$

If the wind is blowing perpendicular to the boundary (*i.e.*, $\varphi = \vartheta$), then the wind flow rate across the boundary is just the wind speed; otherwise, it is flowing across the boundary with a velocity less than the wind speed, the magnitude of which depends on the angular difference between the wind vector and the unit vector normal to the boundary.

Although Equation 3-1 includes lateral/dispersive wind velocity, the equation implemented in TRIM.FaTE for the horizontal air-to-air compartment transfer factor includes only the direct advective wind velocity:

$$T_{Air_Send \rightarrow Air_Rcv}^{adv} = \frac{1}{V_{Air_Send}} \times \sum_{i=1}^n A_i \times (u_i^{(D)}) \quad (\text{TF 3-1})$$

where:

$T_{Air_Send \rightarrow Air_Rcv}^{adv}$	=	advective transfer factor for wind in air from sending (<i>Send</i>) to receiving (<i>Rcv</i>) air compartments (/day);
V_{Send}	=	volume of sending air compartment (m ³);
A_i	=	interfacial area across the i^{th} boundary (m ²); and
$u_i^{(D)}$	=	direct (<i>D</i>) advective wind velocity across the i^{th} boundary (m/day).

The advective transport can occur both horizontally, based on the horizontal component of the wind speed, and vertically, based on the vertical component of the wind speed and the stability class assigned to the air layers. The advective transport Equations 3-1 through 3-5 are hard coded in the main TRIM.FaTE program. The transfer factor in the TRIM.FaTE library passes the information on wind speed and direction to the main TRIM.FaTE program to solve the equations. In initial applications of TRIM.FaTE involving only one layer of air compartments, any chemical transported vertically out of the compartments goes to an air sink.¹ If there is to be no vertical loss of chemical due to vertical advection to the air sink, the user can set the vertical wind speed to zero.

Advective transport in air also can carry the chemical horizontally beyond the boundary of the modeling domain to an air sink for the chemical mass. The transfer factor would be the same as TF 3-1, except that the receiving compartment would be the air sink.

3.2 AIR-TO-SOIL ALGORITHMS

The algorithms describing the transfer of chemical mass between air and soil are presented in Section 5.3.3.

3.3 AIR-TO-SURFACE-WATER ALGORITHMS

Several processes can move chemical mass between the air and surface water compartments, including deposition (Section 3.3.1) and diffusion and volatilization (Section 3.3.2).

3.3.1 DEPOSITION

The algorithms describing the deposition of chemical mass from air to surface water are presented in Section 4.2.1.

3.3.2 DIFFUSION AND VOLATILIZATION

Transfer of chemical between an air compartment and a surface water compartment can occur by advection (*i.e.*, wet and dry deposition of particle-bound chemical and wet deposition of vapor-phase chemical). The advective transfers between air and surface water are described in the surface water chapter (Chapter 4). The diffusion (and volatilization) transfer factors are

¹The single air layer can vary in height (*i.e.*, mixing height) depending on environmental conditions.

described in Section 3.3.2.1. Section 3.3.2.2 includes several methods available to calculate the gas-phase transfer coefficient and the liquid-phase transfer coefficient.

3.3.2.1 Diffusion and Volatilization Transfer Between Air and Surface Water

The following describes the method used for estimating volatilization transfer between air and surface water for any chemical that has a non-zero Henry's law constant. The method is a two-layer resistance model first presented by Whitman (1923) and incorporated into the EPA Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). The following discussion is based primarily on the WASP model documentation.

Volatilization is the movement of a chemical across the air/water interface as the concentration of the dissolved chemical tends toward equilibrium with its vapor-phase concentration. Equilibrium occurs when the partial pressure exerted by the chemical in solution equals the partial pressure of the chemical in the overlying atmosphere. The rate of exchange is proportional to the gradient between the dissolved concentration and the concentration in air.

With the approach described in Whitman (1923), the dissolved concentration in the surface water is assumed to attempt to equilibrate with the gas-phase concentration in the atmosphere via the general equation:

$$\left(\frac{dC_{dissolved}}{dt} \right) = \frac{k_v}{d_w} \times \left(C_{dissolved} - \frac{C_{Air}}{(H / (R \times T))} \right) \quad (\text{Eq. 3-6})$$

where:

- $C_{dissolved}$ = concentration of dissolved chemical (g[chemical]/m³[water]);
- k_v = volatilization transfer rate (m/day);
- d_w = water depth (m), assumed to be generally the same throughout the water body;
- C_{Air} = vapor-phase concentration of chemical in air (g[chemical]/m³[air]);
- H = Henry's law constant for the air-water partitioning of the chemical (Pa-m³/mole);
- R = universal gas constant (8.314 m³-Pa/mol-°K); and
- T = water temperature (°K).

The volatilization transfer rate can range from near 0 to 25 m/day, depending on conditions (Ambrose et al. 1995). Multiplying the above equation by the volume of the surface water compartment, denoted here by V_{SW} , yields:

$$\begin{aligned} \text{Net Flux air to water (g[chemical] / day)} = \\ V_{SW} \times \frac{k_v}{d_w} \times \left(C_{dissolved} - C_{Air} \frac{1}{(H / (R \times T))} \right) \end{aligned} \quad (\text{Eq. 3-7})$$

The term V_{SW}/d_w will be equal to the surface area of the water compartment, if the depth of the water compartment is approximately constant. This area is also the interfacial area between the air and water compartments, so that:

$$\begin{aligned} \text{Net Flux air to water} = \\ A_{SWA} \times k_v \times \left(\frac{\text{Fraction_Mass_Dissolved}}{\text{Volume_Fraction_Liquid}} \times \frac{N_{SW}}{V_{SW}} \right. \\ \left. - \frac{\text{Fraction_Mass_Vapor}}{\text{Volume_Fraction_Vapor}} \times \frac{N_{Air}}{V_{Air}} \times \frac{1}{(H / (R \times T))} \right) \end{aligned} \quad (\text{Eq. 3-8})$$

or, using the notation of transfer factors and Equations 2-81 and 2-80:

$$T_{Air \rightarrow SW}^{dif} = \frac{A_{SWA}}{V_{Air}} \times \frac{k_v}{(H / (R \times T))} \times f_{MV} \quad (\text{TF 3-2})$$

$$T_{SW \rightarrow Air}^{vol} = \frac{A_{SWA}}{V_{SW}} \times k_v \times f_{ML} \quad (\text{TF 3-3})$$

where:

$T_{Air \rightarrow SW}^{dif}$	=	transfer of chemical from air to surface water via diffusion (/day);
A_{SWA}	=	interfacial area between the surface water and air compartments (m ²);
V_{Air}	=	volume of air compartment (m ³);
k_v	=	volatilization transfer rate (m/day) [see below for details];
H	=	Henry's law coefficient for the air/water partitioning of the chemical (Pa-m ³ /mole).
R	=	universal gas constant (8.314 m ³ -Pa/mole-°K);
T	=	water temperature (°K);
f_{MV}	=	fraction of chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the compartment that is gas (<i>i.e.</i> , excluding particles);
$T_{SW \rightarrow Air}^{vol}$	=	transfer of chemical from surface water to air via volatilization (/day);
V_{SW}	=	volume of surface water compartment (m ³); and
f_{ML}	=	fraction of the chemical mass in the water compartment that is dissolved in water divided by the volume fraction of the compartment that is water (<i>i.e.</i> , excluding suspended sediments or algae) (unitless).

The two-layer resistance method assumes that two "stagnant films" are bounded on either side by well mixed compartments. Concentration differences serve as the driving force for volatilization from the water. Pressure differences drive the diffusion from the air layer. From mass balance considerations, it is obvious that the same mass must pass through both films; thus, the two resistances combine in series, so that the conductivity is the reciprocal of the total

resistance. Thus, the volatilization transfer rate is estimated in the current TRIM.FaTE library as:

$$k_v = (R_L + R_G)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T} \right)^{-1} \right]^{-1} \quad (\text{Eq. 3-9})$$

where:

R_L	=	liquid-phase resistance (day/m);
k_L	=	liquid-phase transfer coefficient (m/day);
R_G	=	gas-phase resistance (day/m); and
k_G	=	gas-phase transfer coefficient (m/day).

There is actually yet another resistance involved, the transport resistance between the two interfaces, but it is assumed to be negligible (although this may not be true in very turbulent conditions or in the presence of surface-active contaminants).

The value of k_v , the volatilization transfer rate, or conductivity, depends on the intensity of turbulence in a water body and in the overlying atmosphere. Mackay and Leinonen (1975) have discussed conditions under which the value of k_v is primarily determined by the intensity of turbulence in the water. As Henry's law coefficient increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. As Henry's law coefficient decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

Henry's law coefficient generally increases with increasing vapor pressure of a chemical and generally decreases with increasing solubility of a chemical. Thus, highly volatile low-solubility chemicals are more likely to exhibit mass-transfer limitations in water, and relatively nonvolatile high-solubility chemicals are more likely to exhibit mass transfer limitations in the air. Volatilization is usually of relatively lower magnitude in lakes and reservoirs than in rivers and streams.

In cases where it is likely that the volatilization rate is regulated by the turbulence level in the water phase, estimates of volatilization can be obtained from results of laboratory experiments. As discussed by Mill et al. (1982), small flasks containing a solution of a pesticide dissolved in water that have been stripped of oxygen can be shaken for specified periods of time. The amount of pollutant lost and oxygen gained through volatilization can be measured and the ratio of conductivities (K_{VOG}) for pollutants and oxygen can be calculated. As shown by Tsivoglou and Wallace (1972), this ratio should be constant irrespective of the turbulence in a water body. Thus, if the reaeration coefficient for a receiving water body is known or can be estimated and the ratio of the conductivity for the pollutant to reaeration coefficient has been measured, the pollutant conductivity can be estimated.

The volatilization rate constant is for a temperature of 20°C. It is adjusted for segment temperature using the equation:

$$k_{v,T} = k_{v,20} \times \Theta_v^{T-20} \quad (\text{Eq. 3-10})$$

where:

$k_{v,20}$	=	calculated volatilization transfer rate (m/day) at 20°C;
Θ_v^{T-20}	=	temperature correction factor for volatilization (unitless); and
T	=	water temperature (°C).

3.3.2.2 Calculation of Volatilization Transfer Rates for the Whitman Two-layer Resistance Model

There are a variety of methods for estimating the transfer rates k_G and k_L for stagnant and flowing water bodies, many of which are available in the current TRIM.FaTE library. These methods are summarized in Tables 3-1 and 3-2 at the end of this chapter.

3.4 AIR-TO-PLANT ALGORITHMS

The algorithms describing the transfer of chemical mass between air and plants are presented in Sections 7.2.1 (advection processes) and 7.2.2 (diffusion processes).

3.5 TRANSFORMATIONS AND DEGRADATION

Transformations of chemicals into compounds that will no longer be tracked in TRIM.FaTE (*e.g.*, non-toxic degradation products) are called general degradation processes. In TRIM.FaTE, the degradation of a chemical in air due to all mechanisms that might apply (*e.g.*, oxidation, photolysis) is reflected by the user input for the half-life of the chemical in air. The algorithm relating the degradation rate constant to the chemical half-life in the air compartment is presented in Chapter 2 (Equation 2-64), and the corresponding transfer factor is TF 2-1. The degradation transfer factor moves the chemical mass to a degradation sink.

TRIM.FaTE has the capability to track the newly formed compounds, when they are of particular interest to the user. Transformations of a chemical into another form(s) that is tracked in TRIM.FaTE are named for the processes (*e.g.*, oxidation, methylation, reduction of mercury species). In the TRIM.FaTE air compartments, all transformations are modeled as first-order processes; that is, linear with inventory (*i.e.*, the quantity of chemical contained in a compartment). The rate of mass removal in a first-order transformation is calculated as the product of the total inventory of chemical in the compartment and the transformation rate constant specified in the corresponding transfer factor.

3.6 AIR BOUNDARY CONTRIBUTIONS

The TRIM.FaTE library includes algorithms to allow transport of chemical into the modeling region from the ambient air located outside the modeling area. For many of the

chemicals that will be modeled using TRIM.FaTE, so-called “background” concentrations in the absence of the modeled source(s) are not zero. Trace or higher concentrations of a chemical of interest might be found in ambient air due to natural causes or due to releases from other facilities outside the modeling region.

To model chemical inputs to the modeling region via advection of ambient levels of chemical in air from beyond the boundary of the modeling region in TRIM.FaTE, the user can set a boundary concentration for any outside interface of an air compartment located just inside the boundary of the modeled region. In the TRIM.FaTE definition of properties for each of the outside air volume elements, there is a property called the `BoundaryConcentration_g_per_m3` for which the user may specify an ambient air concentration of the chemical in the absence of the source(s) being modeled.

Chemical mass enters the air compartments located just inside the boundary of the modeling region via an air advection algorithm that incorporates wind speed, wind direction, and the boundary concentration of the chemical (see above). The use of wind speed and wind direction in this algorithm is identical to the approach that is used for the air-to-air advection algorithm.

Note that TRIM.FaTE does not model changes in chemical concentrations in the air external to the modeling region that might occur as a consequence of emissions from the modeled source. Losses of chemical via air advection from the modeling region to areas external to that region are modeled as transfers of the chemical to an air sink.

Table 3-1
Methods for Determining Gas-Phase Transfer Coefficient k_G^a for the
Whitman Two-Layer Resistance Volatilization Model Between Air and Surface Water

Water Body Type	Method	k_G , Gas phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	1*	$k_G = u^* \times \left(\frac{\kappa^{0.33}}{\lambda_2} \right) \times Sc_{air}^{-0.67}$ <p>where:</p> $u^* = \text{the shear velocity (m/day) computed from } u^* = C_d^{0.5} W_{10} \times 86,400$ <p>where:</p> $C_d = \text{drag coefficient (= 0.0011),}$ $W_{10} = \text{wind velocity 10 m above water surface (m/sec), and}$ $86,400 = \text{unit conversion factor (sec/day);}$ $\kappa = \text{von Karmen's constant (= 0.74) (unitless);}$ $\lambda_2 = \text{dimensionless viscous sublayer thickness = (4) (unitless); and}$ $Sc_{air} = \text{air Schmidt Number, computed from } Sc_{air} = \frac{\mu_{air}}{10000 \times D_{air}},$ <p>where:</p> $\mu_{air} = \text{viscosity of air, internally calculated from air temperature (cm}^2\text{/sec),}$ $= \frac{10}{(1.32 + 0.009 T_{airC})},$ <p>where: T_{airC} = air temperature ($^{\circ}\text{C}$), and</p> $D_{air} = \text{diffusivity of chemical in air (m}^2\text{/sec) } = \frac{1.9 \times 10^{-4}}{M_w^{2/3}}$ <p>where: M_w = molecular weight of compound (g/mole).</p>	O'Connor (1983), Ambrose et al. (1995)
Stagnant Pond or Lake	2	<p>See Method (1) for definition of terms.</p> $k_G = 10^{-3} + 0.0462 \times u^* \times Sc_{air}^{-0.67}$	Mackay and Yeun (1983), Ambrose et al. (1995)
Flowing Water or Estuary	1*	Same as Method (1) for stagnant water body.	
Flowing Water or Estuary	2	Same as Method (2) for stagnant water body.	
Flowing Water or Estuary	3*	Input value of 100 m/day.	Ambrose et al. (1995)

^a Used in the calculation of the volatilization transfer rate k_v : $k_v = (R_L + R_G)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T_c} \right)^{-1} \right]^{-1}$.
 * Available in current TRIM.FaTE Library.

Table 3-2
Methods for Determining Liquid-Phase Transfer Coefficient k_L for the
Whitman Two-Layer Resistance Volatilization Model Between Air and Surface Water

Water Body Type	Method	k_L , Liquid phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	1*	$k_L = k_a \times K_{vo}$ where: k_a (user input) = reaeration velocity (m/day); and K_{vo} (user input) = ratio of volatilization rate to reaeration rate (unitless).	Ambrose et al. (1995)
Stagnant Pond or Lake	2*	$k_L = k_g \times (32/M_w)^{0.5}$ where: M_w = molecular weight	Ambrose et al. (1995)
Stagnant Pond or Lake	3*	$k_L = u^* \times \left(\frac{\rho_a}{\rho_w} \right)^{0.5} \times \left(\frac{\kappa^{0.33}}{\lambda_2} \right) \times Sc_w^{-0.67}$ where: u^* = the shear velocity (m/day) computed from $u^* = C_d^{0.5} \times W_{10} \times 86,400$ where: C_d = drag coefficient (= 0.0011), W_{10} = wind velocity 10 m above water surface (m/sec), and $86,400$ = unit conversion factor (sec/day); ρ_a = density of air, internally calculated from air temperature (kg/m ³); ρ_w = density of water, internally calculated from water temperature (kg/m ³); κ = von Karman's constant (= 0.74) (unitless); and λ_2 = dimensionless viscous sublayer thickness (= 4) (unitless). Sc_w = water Schmidt Number, computed from $Sc_w = \frac{\mu_w}{\rho_w \times D_w}$ where: μ_w = viscosity of water, internally calculated from water temperature (kg/m-sec) D_w = diffusivity of chemical in water (m ² /sec) where: M_w = molecular weight of compound (g/mole). $10^{(-3.30233 + 1301/(998.333 + 8.1855(T_w - 20) + 0.00585(T_w - 20)^2))}$, where: T_w = water temperature (°C)	O'Connor (1983), Ambrose et al. (1995)

Table 3-2 (continued)
Methods for Determining Liquid Phase Transfer Coefficient k_L for the Whitman Two-Resistance Volatilization Model
Between Air and Surface Water

Water Body Type	Method	k_L , Liquid phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	4*	$k_L = 10^{-6} + 0.00341 \times u^* \times Sc_w^{-0.5}$ if $u^* > 0.3$ m/s $k_L = 10^{-6} + 0.0144 \times u^{*0.22} \times Sc_w^{-0.5}$ if $u^* < 0.3$ m/s See Method (3) for definition of terms.	Mackay and Yeun (1983), Ambrose et al. (1995)
Flowing Water or Estuary	1*	Same as Method (1) for stagnant water body.	
Flowing Water or Estuary	2	Same as Method (2) for stagnant water body.	
Flowing Water or Estuary	3*	Same as Method (3) for stagnant water body.	
Flowing Water (e.g., stream, river) or Estuary	4*	$k_L = k_a \times K_{vo}$, where: $k_a = 5.349 \times \frac{u^{0.67}}{d_w^{0.85}}$ if $d_w < 0.61$ m $k_a = 8.64 \times 10^{-4} \times \sqrt{\frac{D_w \times u}{d_w}}$ if $d_w \geq 0.61$ m and $(u < 0.518 \text{ m/s or } d_w > 13.584 \times u^{0.29135})$ $k_a = 5.049 \times \frac{u^{0.969}}{d_w^{0.673}}$ else $K_{vo} = \text{input or } = \sqrt{\frac{32}{M_{H_2O}}}$ where: u = velocity of water (m/sec); d_w = water compartment depth (m); D_w = diffusivity of chemical in water (m ² /sec) (= 22E-9 / $M_w^{2/3}$); K_{vo} = input = ratio of volatilization rate to reaeration rate (unitless); and k_a = input = reaeration velocity (m/day).	Covar (1976), Ambrose et al. (1995)

^a Used in the calculation of the volatilization transfer rate k_v : $k_v = (R_L + R_G)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T_K} \right)^{-1} \right]^{-1}$.

* = Available in current TRIM.FaTE Library.